

Oxazole  
288-42-6 | DTXSID70182983

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $3.15 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $2.59 \times 10^{-1}$

**Confidence level:**  $7.99 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Glyoxal

**Measured:**  $1.14 \times 10^{-11}$

**Predicted:**  $1.14 \times 10^{-11}$

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(2E)-3-Phenylprop-2-enal

**Measured:**  $4.80 \times 10^{-11}$

**Predicted:**  $5.31 \times 10^{-11}$

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(E)-Crotonaldehyde

**Measured:**  $3.61 \times 10^{-11}$

**Predicted:**  $3.73 \times 10^{-11}$

Image not found

Crotonaldehyde

**Measured:**  $3.61 \times 10^{-11}$

**Predicted:**  $3.73 \times 10^{-11}$

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2(3H)-Furanone

**Measured:**  $4.45 \times 10^{-11}$

**Predicted:**  $3.74 \times 10^{-11}$